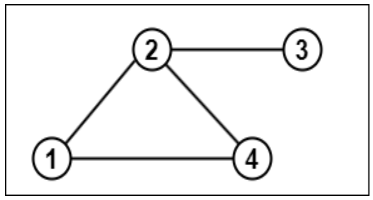
Mid-term Exam (Graph Neural Networks –Fall 2023)

Full Name:
Student ID:

1. Consider an undirected graph G of four nodes given in the following figure. The normalized adjacency matrix is defined as: $\tilde{A} = D^{-1} \cdot A$, where A is the adjacency matrix of G and D is the node degree matrix.
   a) Calculate the matrix $\tilde{A}$
   b) Calculate the 2-step transition probability matrix $\tilde{A}^2$



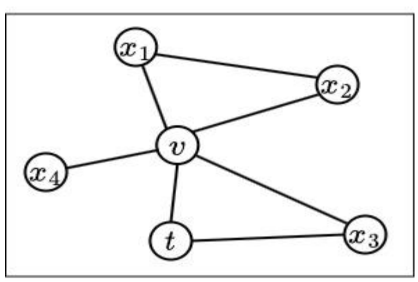
Solutions:

$$A = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix} \qquad \text{D=}\begin{bmatrix} 2 \\ 3 \\ 1 \\ 2 \end{bmatrix}$$

$$\tilde{A} = \frac{A}{D} = \begin{bmatrix} 0 & .5 & 0 & .5 \\ .33 & 0 & .33 & .33 \\ 0 & 1 & 0 & 0 \\ .5 & .5 & 0 & 0 \end{bmatrix}$$

$$\tilde{A}^2 = \tilde{A} \times \tilde{A} = \begin{bmatrix} 0 & .5 & 0 & .5 \\ .33 & 0 & .33 & .33 \\ 0 & 1 & 0 & 0 \\ .5 & .5 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 0 & .5 & 0 & .5 \\ .33 & 0 & .33 & .33 \\ 0 & 1 & 0 & 0 \\ .5 & .5 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0.42 & 0.25 & 0.17 & 0.17 \\ 0.17 & 0.67 & 0 & 0.17 \\ 0.33 & 0 & 0.33 & 0.33 \\ 0.17 & 0.25 & 0.17 & 0.42 \end{bmatrix}$$

2. Consider the Node2vec algorithm with the return parameter $p = 0.2$ and the in-out parameter $q = 0.6$. A walker traversed from node t to node v and now resides at node v. Calculate the transition probabilities from node v to other nodes.



Solutions:

$P(v, x_1) = \frac{1}{q} = \frac{1}{0.6}$

$P(v, x_2) = \frac{1}{q} = \frac{1}{0.6}$

$P(v, x_3) = 1$

$P(v, x_4) = \frac{1}{q} = \frac{1}{0.6}$

$P(v, t) = \frac{1}{p} = \frac{1}{0.2}$

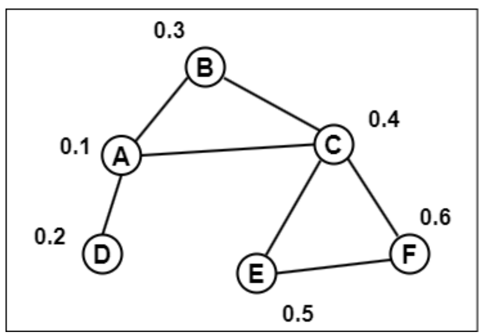
3. Consider an undirected graph G of six nodes A, B, C, D, E, and F given in the following figure. Each node has initial features that are the numbers standing next to it (i.e., the initial feature of node 'A' is $X_A^{(0)} = 0.1$). Assume that the feature of a node i at layer k can be updated as:

$$X_i^{(k)} = F\left(X_i^{(k-1)}, N_i^{(k-1)}\right),$$

where $F(\bullet)$ returns a numeric value that is the mean (average) of its arguments, $N_i^{(k-1)}$ is the set of features of the neighbours of node i at layer $(k-1)$.

a) Calculate the feature of each node at $k = 1$.

b) Calculate the feature of each node at $k = 2$.



Solutions:

$X_A^1 = mean\left(X_A^0 + X_B^0 + X_C^0 + X_D^0\right) = \frac{0.1+0.2+0.3+0.4}{4} = 0.25$

$X_B^1 = mean\left(X_A^0 + X_B^0 + X_C^0\right) = (0.1+0.3+0.4)/3 = 0.27$

$X_C^1 = (0.1+0.3+0.4+0.5+0.6)/5 = 0.38$

$X_D^1 = (0.1+0.2)/2 = 0.15$

$X_E^1 = (0.4+0.5+0.6)/3 = 0.5$

$X_F^1 = (0.4+0.5+0.6)/3 = 0.5$

$$X_A^2 = mean\left(X_A^1 + X_B^1 + X_C^1 + X_D^1\right) = \frac{0.25+0.27+0.38+0.15}{4} = 0.26$$

$$X_B^2 = mean\left(X_A^1 + X_B^1 + X_C^1\right) = (0.25+0.27+0.38)/3 = 0.3$$

$$X_C^2 = (0.25+0.27+0.38+0.5+0.5)/5 = 0.38$$

$$X_D^2 = (0.25+0.15)/2 = 0.2$$

$$X_E^2 = (0.38+0.5+0.5)/3 = 0.43$$

$$X_F^2 = (0.38+0.5+0.5)/3 = 0.46$$

4. Given a graph with an adjacency matrix A and initial node feature matrix $H^{(0)}$ as follows:

$$A = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix} \qquad H^{(0)} = \begin{bmatrix} 0 & 0 \\ 1 & -1 \\ 2 & -2 \\ 3 & -3 \\ 4 & -4 \\ 5 & -5 \end{bmatrix}$$

Assume that the hidden layer of an GCN model of all nodes at layer (k) can be calculated as:

$$H^{(k)} = \sigma\left(A \cdot H^{(k-1)}\right),$$

where $H^{(k)}$ denotes the output at layer k, σ is a ReLU function $\text{ReLU}(x) = \max(0, x)$. Calculate the output of the GCN model at layer $k = 1$.

Solutions:

$$H^1 = \sigma\left(AH^0\right) = \text{ReLU}\left(\begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix} \times \begin{bmatrix} 0 & 0 \\ 1 & -1 \\ 2 & -2 \\ 3 & -3 \\ 4 & -4 \\ 5 & -5 \end{bmatrix}\right) = \text{ReLU}\left(\begin{bmatrix} 6 & -6 \\ 2 & -2 \\ 1 & -1 \\ 9 & -9 \\ 8 & -8 \\ 7 & -7 \end{bmatrix}\right) = \begin{bmatrix} 6 & 0 \\ 2 & 0 \\ 1 & 0 \\ 9 & 0 \\ 8 & 0 \\ 7 & 0 \end{bmatrix}$$